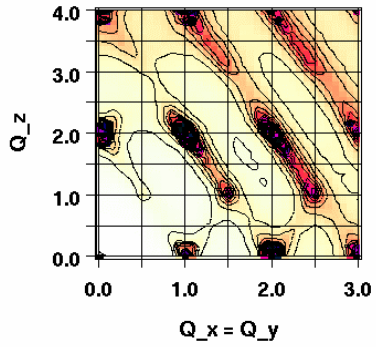
VI.C Atomistic Simulations of Martensitic Transformations

Introduction: The formation of a martensitic phase controls the strength and hardness of carbon steels. The martensitic transformation is a diffusionless, cooperative movement of atoms resulting in a unique microstructure. Martensitic transformations are also responsible for shape memory effects in "smart materials" [e.g., NiTi-alloys]. Materials scientists are studying the formation of martensite in order to understand more about the complexities of how it forms to enable the design of specialized alloys and smart materials. Some important clues in understanding martensite formation come from x-ray studies at high temperatures. These experiments exhibit an unusual streaking pattern which suggest that there is an instability in the material that precedes the actual formation of martensite. The details of the cause of the streaking have been a puzzle for decades. Zirconium was chosen as a model material since, as an element, its martensitic transformation (at 1133 K) is uncomplicated by alloying effects.



Calculated scattering in the < 110> plane

Calculational Notes: The calculations involved molecular dynamics simulations for a model of zirconium with up to 200,000 atoms per unit cell and up to 80,000 time steps for extracting anharmonic lattice dynamics. They used classical embedded atom potentials fit to extensive first principles electronic structure calculations. The calculations ran on the 1024-node Intel Paragon XP/S-150 at ORNL-CCS.

Results: In the figure shown above the calculated x-ray scattering of the high-temperature bcc phase shows a characteristic streaking in the x-ray patterns as observed in experiments. Examination of the x-ray scattering as a function of time shows that the streaking is due to coherent atomic fluctuations toward the low temperature hcp martensitic phase. The picture shown to the left illustrates the microstructure after quenching to below the transformation temperature, with blue atoms separating the three orientationally different types of domains of transformed material.

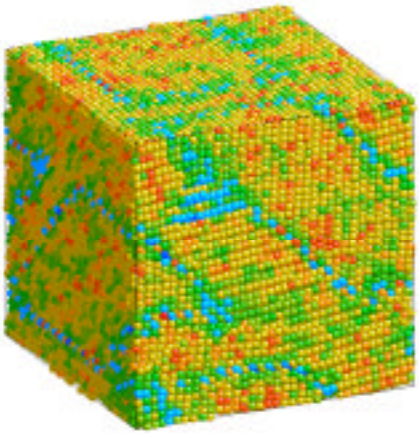


Image of microstructure formation in cubic simulation cell

Significance: This computational exploration demonstrates the potential of realistic atomistic simulations for understanding complex dynamical phenomena; in this case the calculations explained a long outstanding problem in experimental metallurgy. The ability to model phase transformation in metals and alloys, such as the martensite transformation, will enable materials scientists to control the microstructural properties of alloys. The increased computational power of terascale computers will allow detailed studies on more complicated and technologically relevant multi component alloys.